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Determining the scattering cross section from the S matrix

1 Introduction

Consider a general scattering process in which an incident beam particle b with momentum $\vec{p}_b$ strikes a target particle t with momentum $\vec{p}_t$ and produces N final-state particles $i = 1, \ldots, N$ with momenta $\vec{p}_i$.

We will treat the scattering using time-dependent perturbation theory and assume a Hamiltonian of the form

$$H = H_0 + V. \tag{1}$$

Here H_0 is a free-particle Hamiltonian which describes non-interacting incident and outgoing particles. The perturbation V is the source of the scattering. It is assumed to be short range so its effects can be ignored when the particles are far separated. This allows us to use H_0 to describe the motion of the initial and final particles long before and long after the scattering has occurred when the initial state is created and the final state observed.

We begin with an initial H_0 eigenstate, $|\vec{p}_b, \vec{p}_t\rangle$, which is a momentum eigenstate and describes the two initial particles:

$$H_0|\vec{p}_b, \vec{p}_t\rangle = \left(\frac{\vec{p}_b^{\,2}}{2m_b} + \frac{\vec{p}_t^{\,2}}{2m_t}\right)|\vec{p}_b, \vec{p}_t\rangle, \tag{2}$$

and is normalized to a product of delta functions:

$$\langle \vec{p}\,'_b, \vec{p}\,'_t|\vec{p}_b, \vec{p}_t\rangle = \delta^3(\vec{p}\,'_b - \vec{p}_b)\delta^3(\vec{p}\,'_t - \vec{p}_t). \tag{3}$$

Similarly a momentum eigenstate, $|\vec{p}_1, \ldots, \vec{p}_N\rangle$, will be introduced to describe the final state which obeys:

$$\begin{aligned} H_0|\vec{p}_1, \ldots, \vec{p}_N\rangle &= \left(\sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m_i}\right)|\vec{p}_1, \ldots, \vec{p}_N\rangle & (4)\\ \langle \vec{p}\,'_1, \ldots, \vec{p}\,'_N|\vec{p}_1, \ldots, \vec{p}_N\rangle &= \prod_{i=1}^{N}\left(\delta^3(\vec{p}\,'_i - \vec{p}_i)\right). & (5)\end{aligned}$$

Next to specify the dynamics which determines the scattering we will define the scattering matrix S using the interaction picture time development operator

$$S = \lim_{\substack{t_i \to -\infty \\ t_f \to \infty}} T\left\{e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} V_I(t)dt}\right\}. \tag{6}$$

We will assume that physics described by S is translationally invariant in both time and space so that energy and momentum are conserved. In this case it is very useful to extract explicit delta functions which enforce energy and momentum conservation from the matrix elements of S and to define the T matrix as follows:

$$\langle\vec{p}_1,\ldots,\vec{p}_N|S-I|\vec{p}_b,\vec{p}_t\rangle = i\delta(E_f-E_i)\delta^3(\vec{P}_f-\vec{P}_i)\langle\vec{p}_1,\ldots,\vec{p}_N|T|\vec{p}_b,\vec{p}_t\rangle \tag{7}$$

where:

$$E_i = \frac{\vec{p}_b^{\,2}}{2m_b}+\frac{\vec{p}_t^{\,2}}{2m_t}, \qquad E_f=\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2m_i}, \tag{8}$$

while

$$\vec{P}_i=\vec{p}_b+\vec{p}_t, \qquad \vec{P}_f=\sum_{i=1}^{N}\vec{p}_i. \tag{9}$$

The $-I$ appearing in the matrix element on the left-hand side of Eq. (7) removes that component of the time development which involves no scattering.

The requirement of translational symmetry in space implies that when we want to study scattering from a fixed potential, we must introduce a particle of mass m_t which is the source of that potential and then take the limit $m_t\to\infty$. As m_t increases, the recoiling target particle will carry a fixed transferred momentum $\vec{p}_t^{\,\prime}$ but its energy, $\vec{p}_t^{\,\prime 2}/2m_t$ will vanish for large m_t so the scattering will be the same as the scattering from a fixed potential.

Using the quantities just defined we can write down what will be the final result from this discussion, an explicit formula for the scattering cross section:

$$d\sigma=\frac{(2\pi\hbar)^2}{v_b}\left\{\prod_{i=1}^{N}(\Delta p_i)^3\right\}\left|\langle\vec{p}_1,\ldots,\vec{p}_N|T|\vec{p}_b,\vec{p}_t\rangle\right|^2\delta(E_f-E_i)\delta^3(\vec{P}_f-\vec{P}_i), \tag{10}$$

where v_b is the velocity of the incoming beam particle. When multiplied by the flux F of particles crossing the location of the target per unit time and unit area, $d\sigma F$, will give the differential rate of scattering into final state momenta $\vec{p}_i,\ldots\vec{p}_N$ each of which lies in the corresponding volume $(\Delta p_i)^3$ around an average final momentum. Just as in the simpler example of Fermi's Golden Rule, the energy and momentum delta functions must be eliminated by performing an integral over four of the final state variables. These are typically the 3-momentum of one final particle and the kinetic energy of another. This is a very useful formula which can be used in both non-relativistic and relativistic scattering problems. It is limited by its reliance on perturbation theory since we can typically evaluate the matrix elements of the operator S, given in Eq. (6), only in low-order perturbation theory. However, we can consider interesting cases for H_0 which could include those parts of the potential that are needed to combine some of the particles into bound states. This would allow the scattering of a positron from a hydrogen atom for example.

We will now give a derivation of this formula.

2 Derivation

We adopt a detailed strategy for specifying the wave packets for the beam and target particles which are initially far apart but then come together and are assumed to overlap at $\vec{r} = 0$ and $t = 0$, the position and time of scattering. Likewise the N final-state wave functions are assumed to have been localized at $\vec{r} = 0$ at $t = 0$ but to fly apart and at large t to be outgoing wave packets with reasonably well-defined momenta.

Since we do not want to solve for the eigenstates of the complete Hamiltonian H in order to set up the scattering problem, we adopt the following procedure. We begin by constructing wave functions for the $N + 2$ particles being studied which are each single-particle eigenstates of the free-particle Hamiltonian H_0 and are concentrated in position space at the origin $\vec{r} \approx 0$ where the scattering is presumed to take place. This seems illogical because this is precisely the region where scattering must take place and the scattering potential V is important. However, we will take the product of the free-particle beam and target wave functions and evolve them backward in time using H_0 to an early initial time $t_i \ll 0$ when they are far apart and use this as our initial state specified at time t_i. We will then propagate this state forward in time with the full Hamiltonian H insuring that V has its proper effect when the particles collide at $t \approx 0$. The overlapping product of possible final state eigenstates of H_0 is similarly evolved forward in time using H_0 to a far future final time $t_f \gg 0$. This state with the particles now far separated is both an eigenstate of H and H_0 and a physically sensible final state into which we will calculate the probability of scattering.

Following this approach, the beam and target wave functions are taken to be wave packets localized at $\vec{r} \approx 0$: $\psi_b(\vec{r}_b)$ and $\psi_t(\vec{r}_t)$. In momentum space, these wave functions, $\widetilde{\psi}_b(\vec{p}_b)$ and $\widetilde{\psi}_t(\vec{p}_t)$, are assumed to be peaked in momentum around the average values $\vec{p}_b \approx \vec{\bar{p}}_b$ and $\vec{p}_t \approx \vec{\bar{p}}_t$. We will use $|i\rangle$ to represent this state. The N scattered wave functions $F(\vec{r}_i)$ are similarly taken to be wave packets localized at $\vec{r} = 0$. In momentum space, $\widetilde{F}(\vec{p}_i)$ are assumed to be simple characteristic functions of the momentum $\vec{p}_i$, centered about the average value $\vec{\bar{p}}_i$:

$$\widetilde{F}(\vec{p}_i) = \begin{cases} \frac{1}{(\Delta p_i)^{3/2}} & \bar{p}_i^a - \frac{\Delta p_i}{2} \leq p_i \leq \bar{p}_i^a + \frac{\Delta p_i}{2}, \quad 1 \leq a \leq 3 \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

The product of these N states is denoted $|f\rangle$ The actual initial and final states will be obtained by propagating ψ_b and ψ_t to $t_i \ll 0$ and the F_i to $t_f \gg 0$.

Thus, we can easily express the probability for a transition from our initial state to our final state as:

$$P_{i\to f} = \lim_{\substack{t_i \to -\infty \\ t_f \to \infty}} \left| \left[\langle f| e^{+iH_0 t_f/\hbar} \right] e^{-iH(t_f - t_i)/\hbar} \left[e^{-iH_0 t_i/\hbar} |i\rangle \right] \right|^2. \tag{12}$$

If we recall that the exact time development operator $e^{-iH(t_f - t_i)}$ can be written using the interaction picture time development operator as:

$$e^{-iH(t_f - t_i)} = e^{-iH_0 t_f} T \left\{ e^{-\frac{i}{\hbar} \int_{t_i}^{t_f} V_I(t) dt} \right\} e^{iH_0 t_i} \tag{13}$$

we can recognize Eq. (12) as the matrix element of the interaction picture time-development operator:

$$P_{i\to f} = \lim_{\substack{t_i\to-\infty \\ t_f\to\infty}} \left| \langle f|T\left\{ e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} V_I(t)dt} \right\}|i\rangle \right|^2 \tag{14}$$

$$= \left|\langle f|S|i\rangle\right|^2. \tag{15}$$

If we presume that the final state does not overlap with the initial state then we can subtract the identify from S in Eq. (15) and substitute our definition of the T matrix from Eq. (7) and obtain the result:

$$P_{i\to f} = \left| \left\{ \prod_{i=1}^{N} \int d^3p_i \int d^3p_b \int d^3p_t \right\} \left\{ \prod_{j=1}^{N} \widetilde{F}(p_j)^* \right\} \right. \tag{16}$$

$$\left. \langle \vec{p}_1 \ldots \vec{p}_N|T|\vec{p}_b,\vec{p}_t\rangle\ \widetilde{\psi}_b(\vec{p}_b)\widetilde{\psi}_t(\vec{p}_t)\ \delta(E_f-E_i)\delta^3(\vec{P}_f-\vec{P}_i)| \right|^2.$$

So far we have made no approximations. To make further progress we must make assumptions about what we are trying to determine. The most important is the assumption that as we perform the $3(N+2)$ dimensional integrals to evaluate Eq. (16) the T matrix element $\langle \vec{p}_1 \ldots \vec{p}_N|T|\vec{p}_b,\vec{p}_t\rangle$ can be treated as a constant. This important physical assumption dictates the type of scattering problem we are tying to solve. We are not interested in seeing the effects of interference between the scattering of components of initial or final states which have different momenta and experience different scattering because of their different momenta. We have decided to prepare initial states and determine final states whose momenta are sufficiently precise that the matrix elements of T can be treated as a constant.

With this assumption, Eq. (16) simplifies enormously:

$$P_{i\to f} = C_{f,i}\left|\langle \vec{\bar{p}}_1 \ldots \vec{\bar{p}}_N|T|\vec{\bar{p}}_b,\vec{\bar{p}}_t\rangle|\right|^2 \tag{17}$$

where the kinematic function $C_{f,i}$ is completely independent of the physics which is causing the scattering and can be determined independent of the scattering mechanism!

Next we must determine $C_{f,i}$ which is given by

$$C_{f,i} = \left| \left\{ \prod_{i=1}^{N} \int d^3p_i \int d^3p_b \int d^3p_t \right\} \left\{ \prod_{j=1}^{N} \widetilde{F}(p_j)^* \right\} \right. \tag{18}$$

$$\left. \cdot\widetilde{\psi}_b(\vec{p}_b)\widetilde{\psi}_t(\vec{p}_t)\ \delta(E_f-E_i)\delta^3(\vec{P}_f-\vec{P}_i)| \right|^2.$$

There are surely many strategies which should lead to the same final result for the function $C_{f.i}$. Our approach will be to first assume that the scattered momenta are determined very accurately so that when evaluating the $3N$ integrals of the final momenta that appear in Eq. (18) we can treat the integrand, not including the final-state wave functions $\widetilde{F}_i(\vec{p}_i)$, as a constant and factor out these integrals over the functions $\widetilde{F}_i(\vec{p}_i)$:

$$\begin{aligned} C_{f,i} &= \left|\left\{\prod_{i=1}^{N}\int d^3p_i\right\}\left\{\prod_{j=1}^{N}\widetilde{F}(p_j)^*\right\}\right|^2 && (19) \\ &\quad \cdot\left|\int d^3p_b\int d^3p_t\widetilde{\psi}_b(\vec{p}_b)\widetilde{\psi}_t(\vec{p}_t)\ \delta(\overline{E}_f - E_i)\delta^3(\vec{\overline{P}}_f - \vec{P}_i)|\right|^2 \\ &= \left\{\prod_{i=1}^{N}(\Delta p_i)^3\right\}\left|\int d^3p_b\int d^3p_t\widetilde{\psi}_b(\vec{p}_b)\widetilde{\psi}_t(\vec{p}_t)\ \delta(\overline{E}_f - E_i)\delta^3(\vec{\overline{P}}_f - \vec{P}_i)|\right|^2 . && (20) \\ &= \left\{\prod_{i=1}^{N}(\Delta p_i)^3\right\}D_{f,i}(\overline{E}_f, \vec{\overline{P}}_f) && (21) \end{aligned}$$

where the second equation comes from evaluating the first factor on the right-hand side of Eq. (19) by performing a simple integral over the functions $F_i(\vec{p}_i)$ defined in Eq. (5).

Note that when separating the expression for $C_{f,i}$ given in Eq. (18) into two factors to obtain Eq. (19) the dependence of the second factor of the integrand on the N final-state integration variables $\vec{p}_i$ enters only through the functions E_f and $\vec{P}_f$ which, in the approximation that the $\vec{p}_i$ can be replaced by their average values $\vec{\overline{p}}_i$, can themselves be replaced by:

$$\overline{E}_f = \sum_{i=1}^{N}\frac{(\vec{\overline{p}}_i)^2}{2m_i}, \quad \vec{\overline{P}}_f = \sum_{i=1}^{N}\vec{\overline{p}}_i . \qquad (22)$$

Thus, our final task is to determine the function $D_{f,i}(\overline{E}_f, \vec{\overline{P}}_f)$ defined in Eq. (21):

$$D_{f,i}(\overline{E}_f, \vec{\overline{P}}_f) = \left|\int d^3p_b\int d^3p_t\widetilde{\psi}_b(\vec{p}_b)\widetilde{\psi}_t(\vec{p}_t)\ \delta(\overline{E}_f - E_i)\delta^3(\vec{\overline{P}}_f - \vec{P}_i)|\right|^2 .. \qquad (23)$$

We begin by evaluating the integral over the target momentum $\vec{p}_t$ using the delta function:

$$\delta^3(\vec{\overline{P}}_f - \vec{P}_i) = \delta^3(\vec{\overline{P}}_f - \vec{p}_b - \vec{p}_t) \qquad (24)$$

to fix $\vec{p}_t$ to obtain

$$D_{f,i}(E_f, \vec{P}_f) = \left|\int d^3p_b\,\widetilde{\psi}_b(\vec{p}_b)\widetilde{\psi}_t\left(\vec{P}_f - \vec{p}_b\right)\ \delta\left(E_f - \frac{(\vec{p}_b)^2}{2m_b} - \frac{(\vec{P}_f - p_b)^2}{2m_t}\right)\right|^2 , \qquad (25)$$

where we have dropped the bars on the averaged final-state variables to reduce complexity and written an explicit formula for the dependent variable E_i.

The final step in simplifying the function $D_{f,i}(E_f, \vec{P}_f)$ is to choose the z-direction to correspond to that of the average beam momentum $\vec{\overline{p}}_b$ and separate the integral over the beam momentum into its z- and transverse components: p_b^z and $\vec{p}_b^{\perp}$ and then to use the energy delta function to fix the value of p_b^z:

$$D_{f,i}(E_f, \vec{P}_f) \tag{26}$$

$$= \left| \int dp_b^z \, d^2\vec{p}_b^{\,\perp} \, \widetilde{\psi}_b(\vec{p}_b) \widetilde{\psi}_t \left(\vec{P}_f - \vec{p}_b \right) \, \delta \left(E_f - \frac{(p_b^z)^2 + (\vec{p}_b^{\,\perp})^2}{2m_b} - \frac{(\vec{P}_f - p_b)^2}{2m_t} \right) \right|^2$$

$$= \left| \int d^2\vec{p}_b^{\,\perp} \, \widetilde{\psi}_b(\vec{p}_b^{\,\perp}, p_b^z(E_f)) \widetilde{\psi}_t \left(\vec{P},_f^{\perp} - \vec{p}_b^{\,\perp}, P_f^z - \vec{p}_b^z(E_f) \right) \frac{1}{v_b} \right|^2, \tag{27}$$

Where the function $p_b^z(E_f)$ is determined by energy conservation, the requirement that the argument of the delta function in the integrand of Eq. (26) vanish:

$$p_b^z(E_f) = \sqrt{2m_b E_f}. \tag{28}$$

In obtaining Eq. (26) we have dropped the $\vec{p}_b^{\,\perp}$ variable from the energy of the beam particle (assuming that it is small), assumed that the energy of the target particle, now given by $(\vec{P}_f - \vec{p}_b)^2/2m_t$ can also be neglected and recognized that when integrating the delta function of energy over the variable p_b^z we will obtain the Jacobean factor $dp_b^z/dE_b = 1/v_b$ where v_b is the velocity of the beam particle.

In order to further simply this expression for the function $D_{f,i}(E_f, \vec{P}_f)$ we will assume that the momentum of the beam and target particles is sufficiently precisely known that $D_{f,i}(E_f, \vec{P}_f)$ will be sharply peaked about values of its arguments which conserve energy and momentum so that we can write

$$D_{f,i}(E_f, \vec{P}_f) = d_{f,i} \, \delta \left(E_f - \frac{\bar{\vec{p}}_b^{\,2}}{2m_b} \right) \delta^3 \left(\vec{P}_f - \bar{\vec{p}}_b \right). \tag{29}$$

and evaluate $d_{f,i}$ from the integral:

$$d_{f,i} = \int dE_f d^3P_f D_{f,i}(E_f, \vec{P}_f) \tag{30}$$

$$= \int dE_f d^3P_f \left| \int d^2\vec{p}_b^{\,\perp} \, \widetilde{\psi}_b(\vec{p}_b^{\,\perp}, p_b^z(E_f)) \widetilde{\psi}_t \left(\vec{P},_f^{\perp} - \vec{p}_b^{\,\perp}, P_f^z - \vec{p}_b^z(E_f) \right) \frac{1}{v_b} \right|^2. \tag{31}$$

We can transform this into a more physical expression by using two theorems from Fourier analysis, Parseval's theorem:

$$\int dx |\psi(x)|^2 = \int dp |\widetilde{\psi}(p)|^2 \tag{32}$$

and the convolution theorem:

$$\psi_1(x)\psi_2(x) = \sqrt{2\pi\hbar} \int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \int dp' \widetilde{\psi}_1(p') \widetilde{\psi}_2(p - p') \tag{33}$$

which states the when multiplied by $\sqrt{2\pi\hbar}$ the Fourier transform of the convolution of two functions is equal to the product of their Fourier transforms. Here the functions $\psi(x)$ and $\widetilde{\psi}(p)$ are related by the conventional symmetric Fourier transform:

$$\psi(x) = \int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \widetilde{\psi}(p). \tag{34}$$

We first change integration variables in Eq. (36) from E_f to p_b^z, acquiring a factor for v_b from the $dE_f = (dE_f/dp_b^z)dp_b^z = v_b dp_b^z$. Next we shift the integration variable P_f^z to $p_t^z = P_f^z - p_b^z$ to obtain:

$$d_{f,i} \;=\; \int dp_b^z dp_t^z d^2 P_f^\perp \left| \int d^2 \vec{p}_b^{\,\perp}\, \widetilde{\psi}_b(\vec{p}_b^{\,\perp}, p_b^z) \widetilde{\psi}_t \left(\vec{P}_{,f}^{\perp} - \vec{p}_b^{\,\perp}, p_t^z \right) \frac{1}{v_b} \right|^2 . \tag{35}$$

We can then use Parseval's theorem twice. First to replace the p_b^z integral of the modulus-squared of the momentum-space beam wave function by the corresponding integral over the beam position x_b^z of the modulus-squared of the position-space beam wave function. A similar mometum- to position-space transformation can be performed for the p_t^z integration. Since we are doing this only for the two z arguments of the beam and target wave functions we will adopt the unconventional notation of placing the $\widetilde{}$ over the specific arguments instead of the entire function. The result is:

$$d_{f,i} \;=\; \int dz_b dz_t d^2 P_f^\perp \left| \int d^2 \vec{p}_b^{\,\perp}\, \psi_b(\widetilde{\vec{p}^{\,\perp}}_b, z_b) \psi_t \left(\widetilde{\vec{P}_f^{\perp} - \vec{p}_b^{\,\perp}}, z_t \right) \frac{1}{v_b} \right|^2 . \tag{36}$$

Finally the convolution theory is used to recognize the integral

$$\int dp_b^\perp \psi_b(\widetilde{\vec{p}^{\,\perp}}_b, z_b) \psi_t \left(\widetilde{\vec{P}_{,f}^{\perp} - \vec{p}_b^{\,\perp}}, z_t \right) \tag{37}$$

as $2\pi\hbar$ times the Fourier transform of the product

$$\psi_b(\vec{x}_f^{\,\perp}, z_b) \psi_t \left(\vec{x}_f^{\,\perp}{}_b^{\perp}, z_t \right) . \tag{38}$$

Since we are squaring the modulus of this wave function and integrating over the corresponding momentum space variable $\vec{P}_f^\perp$, we can again apply Parseval's theorem and instead integrate over the position space variable $\vec{x}^\perp$ to obtain:

$$d_{f,i} = \frac{(2\pi\hbar)^2}{v_b} \int dz_t \int dz_b \int d^2 \vec{x}^{\,\perp} |\psi_b(\vec{x},^{\perp}, x_b^z)|^2 |\psi_t(\vec{x}^{\,\perp}, x_t^z)|^2 . \tag{39}$$

As suggested by Fig. 1, this combination of wave functions is precisely the probability per unit area that the beam particle and the target particle pass over each other. The scattering cross section is the quantity with units of area which multiplies this probability per unit area to give the probability of scattering. Thus, we can combine Eqs. (17), (21), (29) and (39) to obtain the desired expression for the cross section:

$$d\sigma = \frac{(2\pi\hbar)^2}{v_b} \left\{ \prod_{i=1}^{N} (\Delta p_i)^3 \right\} \delta \left(E_f - \frac{\vec{p}_b^{\,2}}{2m_b} \right) \delta^3 \left(\vec{P}_f - \vec{p}_b \right) \left| \langle \vec{p}_1 \ldots \vec{p}_N | T | \vec{p}_b, \vec{p}_t \rangle \right|^2 \tag{40}$$

which is our target equation, anticipated in Eq. (10).

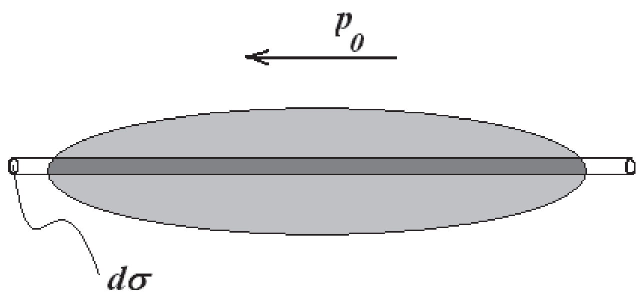

Figure 1: The large shaded area represents the beam wave function $\psi_b(\vec{r}_b)$ at the time of scattering while the darker, thin narrow tube represents the volume swept out by a small hypothetical area $\Delta\sigma$ through which the beam particle must pass for the scattering to occur. This small area would be located at the target position $\vec{r}_t$ and the probability of scattering should include a factor of the modulus squared of the target wave function, $|\psi_t(\vec{x}_t)|^2$, and finally the integral over $\vec{x}_t$ performed. The result, proportional to $\Delta\sigma$ should be the probability of scattering so the coefficient of the expression given by right-hand side of Eq. (39) (including the factor of $(2\pi\hbar)^2/v_b$ in that coefficient) will determine this hypothetical area $\Delta\sigma$.